Unit 2: Energetics, Group Chemistry, Halogenoalkanes and Alcohols

Topic 6: Energetics

Students will be assessed on their ability to:
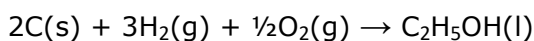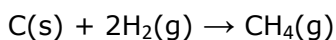
6.1	know that the enthalpy change, ΔH, is the heat energy change measured at constant pressure and that standard conditions are 100 kPa and a specified temperature, usually 298 K
	Enthalpy is a measure of the total energy of a system **Enthapy change** (ΔH) is the heat energy change measured at constant pressure and in standard conditions (100 kPa and a specific temperature, usually 298 K)
6.2	know that, by convention, exothermic reactions have a negative enthalpy change and endothermic reactions have a positive enthalpy change
	Exothermic: heat energy is transferred from the system to surroundings Exothermic reactions have a negative enthalpy change Endothermic: heat energy is transferred from surroundings to system Endothermic reactions have a positive enthalpy change
6.3	be able to construct and interpret enthalpy level diagrams, showing exothermic and endothermic enthalpy changes
	 Exothermic: ΔH is negative Endothermic: ΔH is positive
6.4	know the definition of standard enthalpy change of: i reaction, $\Delta_r H$: the enthalpy change which occurs when equation quantities of materials react under standard conditions ii formation, $\Delta_f H$: the enthalpy change measured at 100kPa and a specified temperature, usually 298K, when one mole of a substance is formed from its elements in their standard states iii combustion, $\Delta_c H$: the enthalpy change measured at 100kPa and a stated temperature, usually 298K, when one mole of a substance is completely burned in oxygen iv neutralisation, $\Delta_{neut} H$: the enthalpy change measured at 100kPa and a stated temperature, usually 298K, when one mole of water is produced by the neutralization of an acid with an alkali v atomisation, $\Delta_{at} H$: the enthalpy change measured at a stated temperature, usually 298K, and 100kPa when one mole of gaseous atoms is formed from an element in its standard state

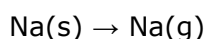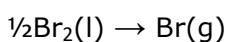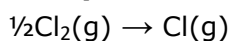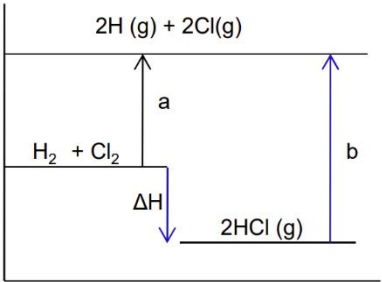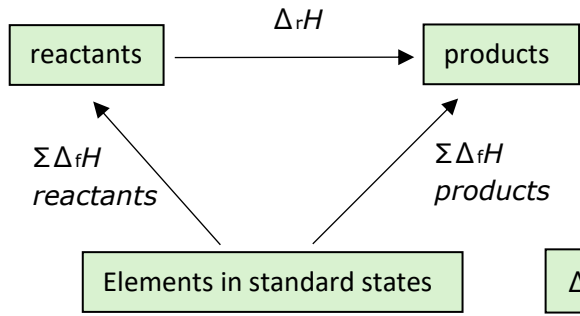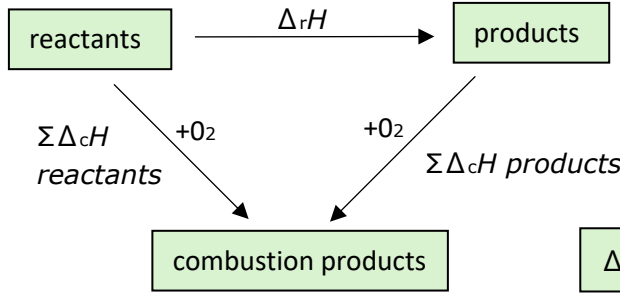|	
	Δ_rH: the enthalpy change which occurs **when equation quantities of materials react under standard conditions**
	Δ_fH: the enthalpy change measured at 100kPa and a specified temperature, usually 298K, **when one mole of a substance is formed from its elements in their standard states** Common examples: $C(s) + 2H_2(g) \rightarrow CH_4(g)$ $2C(s) + 3H_2(g) + \frac{1}{2}O_2(g) \rightarrow C_2H_5OH(l)$
	Δ_cH: the enthalpy change measured at 100kPa and a stated temperature, usually 298K, **when one mole of a substance is completely burned in oxygen (always exothermic)**
	$\Delta_{neut}H$: the enthalpy change measured at 100kPa and a stated temperature, usually 298K, **when one mole of water is produced by the neutralization of an acid with an alkali (always exothermic)**
	$\Delta_{at}H$: the enthalpy change measured at a stated temperature, usually 298K, and 100kPa **when one mole of gaseous atoms is formed from its elements in their standard state (always endothermic)** Common examples: $\quad\quad\quad \frac{1}{2}Cl_2(g) \rightarrow Cl(g)$ $\frac{1}{2}Br_2(l) \rightarrow Br(g)$ $Na(s) \rightarrow Na(g)$
	You can write standard conditions instead of 298K, 100kPa but it's better to write both
6.5	be able to use experimental data to calculate: i energy transferred in a reaction recalling and using the expression: **energy transferred (J) =** **mass (g) × specific heat capacity (J g^{-1} °C^{-1}) × temperature change (°C)** ii enthalpy change of the reaction in kJ mol^{-1} *This will be limited to experiments where substances are mixed in an insulated container and combustion experiments using a suitable calorimeter.*
	For a reaction in solution, we can use:

m is the mass of solution

n is the amount in moles of the limiting reagent

$$Q = mc\,\Delta T$$

$$\Delta H = \frac{Q}{n}$$

6.6	know Hess's Law and be able to apply it to:
	i constructing enthalpy cycles
	ii calculating enthalpy changes of reaction using data provided, or data selected from a table or obtained from experiments
	Hess's Law states that the total enthalpy change of a reaction is independent of the route (path) taken in converting reactants into products, provided that the initial and final conditions are the same in each case

2H (g) + 2Cl(g)

a

$H_2 + Cl_2$

b

ΔH

2HCl (g)

On an energy level diagram the directions of the arrows can show the different routes a reaction can proceed by

In this example one route is arrow '**a**'
The second route is shown by arrows **ΔH** plus arrow '**b**'

So **a = ΔH + b**
And rearranged
ΔH = a - b

Hess's Law is often used to calculate enthalpy change for reactions that cannot be determined directly by experiments (mostly enthalpy changes of formation)
Instead, alternative reactions are carried out that can be measured experimentally |
| | **In general, you can use this enthalpy cycle to calculate enthalpy changes of reaction from enthalpy changes of formation**

Δ_rH

reactants → products

$\Sigma \Delta_fH$ reactants $\Sigma \Delta_fH$ products

Elements in standard states

$\Delta_rH= \Sigma \Delta_fH \text{ products} - \Sigma \Delta_fH \text{ reactants}$ |
| | **In general, you can use this enthalpy cycle to calculate enthalpy changes of reaction from enthalpy changes of combustion**

Δ_rH

reactants → products

$\Sigma \Delta_cH$ reactants $+O_2$ $+O_2$ $\Sigma \Delta_cH$ products

combustion products

$\Delta_rH= \Sigma \Delta_cH \text{ reactants} - \Sigma \Delta_cH \text{ products}$ |
| 6.7 | **CORE PRACTICAL 2**
Determination of the enthalpy change of a reaction using Hess's Law. |

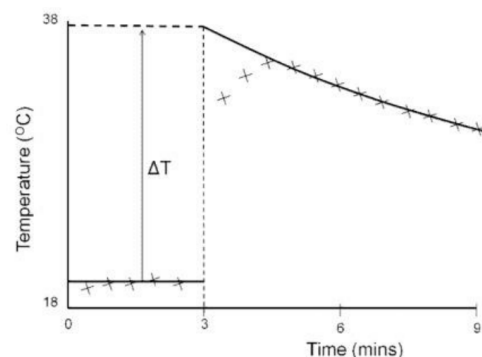| 6.8	be able to evaluate the results obtained from experiments and comment on sources of error and uncertainty and any assumptions made in the experiments
	Students will need to consider experiments where substances are mixed in an insulated container and combustion experiments using, for example, a spirit burner and be able to draw suitable graphs and use cooling curve corrections.
	## Calorimetric Method

General method
- washes the equipment (cup and pipettes etc) with the solutions to be used
- dry the cup after washing
- put polystyrene cup in a beaker **for insulation and support**
- Measure out desired volumes of solutions with volumetric pipettes and transfer to insulated cup
- clamp thermometer into place making sure the thermometer bulb is immersed in solution
- measure the initial temperatures of the solution or both solutions if 2 are used. Do this every minute for 2-3 minutes
- At minute 3 transfer second reagent to cup. If a solid reagent is used then add the solution to the cup first and then add the solid weighed out on a balance.
- If using a solid reagent then use 'before and after' weighing method
- stirs mixture **(ensures that all of the solution is at the same temperature)**
- Record temperature every minute after addition for several minutes

If the reaction is slow then the exact temperature rise can be difficult to obtain as cooling occurs simultaneously with the reaction

To counteract this we take readings at regular time intervals and extrapolate the temperature curve/line back to the time the reactants were added together.

We also take the temperature of the reactants for a few minutes before they are added together to get a better average temperature. If the two reactants are solutions then the temperature of both solutions need to be measured before addition and an average temperature is used.

Errors in this method

- energy transfer from surroundings (usually loss)
- approximation in specific heat capacity of solution. The method assumes all solutions have the heat capacity of water.
- neglecting the specific heat capacity of the calorimeter- we ignore any energy absorbed by the apparatus.
- reaction or dissolving may be incomplete or slow.
- Density of solution is taken to be the same as water.

Calculating the enthalpy change of reaction, ΔH_r from experimental data

General method
1. Using **q= m x c$_p$ x ΔT** calculate energy change for quantities used
2. Work out the moles of the reactants used
3. Divide q by the number of moles of the reactant not in excess to give Δ**H**
4. Add a sign and unit (divide by a thousand to convert Jmol^{-1} to kJmol^{-1}

The heat capacity of water is 4.18 J g^{-1}K^{-1}. In any reaction where the reactants are dissolved in water we assume that the heat capacity is the same as pure water.

Also assume that the solutions have the density of water, which is 1g cm^{-3}. Eg 25cm^3 will weigh 25 g

6.9	understand the terms 'bond enthalpy' and 'mean bond enthalpy', and be able to use bond enthalpies to calculate enthalpy changes, understanding the limitations of this method
	Bond enthalpy is *the enthalpy change when one mole of a specific bond in the gaseous state is broken* **Mean bond enthalpy** is *the average enthalpy change when one mole of a specific (covalent) bond in the gaseous state averaged over many different molecules, is broken* - Mean bond enthalpy is more often used because the bond enthalpy of specific bonds varies with its environment - To calculate enthalpy changes from bond enthalpies, we can use: $\Delta_r H = \Sigma(\text{bonds broken in reactants}) - \Sigma(\text{bonds formed in products})$
6.10	be able to calculate mean bond enthalpies from enthalpy changes of reaction
6.11	understand that bond enthalpy data gives some indication about which bond will break first in a reaction, how easy or difficult it is and therefore how rapidly a reaction will take place at room temperature
	Bond enthalpy data gives some indication about which bond will break first in a reaction, how easy or difficult it is and therefore how rapidly a reaction will take place at room temperature - **Bonds with high bond enthalpy require more energy to break** them so reactions are more likely to require heating and/or catalyst - **Bond with low bond enthalpy require less energy to break** them so are easier to break and thus, more likely to break first in a reaction and is more likely to take place at room temperature
	Further suggested practicals: i the enthalpy change for the decomposition of calcium carbonate using the enthalpy changes of reaction of calcium carbonate and calcium oxide with hydrochloric acid ii the enthalpy change of combustion of an alcohol iii the enthalpy change of the reaction between zinc and copper(II) sulfate solution iv the enthalpy of hydration of anhydrous copper(II) sulfate